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Thermal and mechanical non-equilibrium effects on turbulent flows: fundamental studies of energy exchanges through direct numerical simulations, molecular simulations and experiments

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Abstract

Utilizing internal energy exchange for intelligent control of basic fluid dynamic processes is of direct relevance to AFOSR scientific objectives especially for turbulence flows. The very limited work on the subject suggest strong interactions between thermal non-equilibrium (TNE) and turbulence. This project aimed at both advancing our understanding of the effect of thermal and mechanical non-equilibrium on compressible turbulence and proposing new technological advances in the strategies to generate and control turbulence. Due to the intrinsic multidisciplinary nature of the scientific problem, a combination of state-of-the-art massive direct numerical simulations (DNS), detailed molecular dynamics simulations and novel laser based experimental approaches were developed to explore the detailed physics at levels of fidelity and at a range of parameters not previously possible. A new concept to generate turbulence was studied using TNE via photoexcitation of seeded molecules which can be used to study the specific mechanisms in which TNE modifies turbulence. This technique, which has the advantage of allowing the selection of molecular species to control the degree and mode of TNE, ease of changing grid geometry and initial perturbation and has the potential to revolutionize turbulence studies in high-speed flows, has been investigated numerically and experimentally. In this project we have produced (i) new databases (numerical and physical) and analyses leading to new understanding of the intricate interactions between thermal and mechanical non-equilibrium and the role thereof on the transport of turbulence (ii) development and characterization of a novel "laser grid" concept based on photoexcitation to generate turbulence (iii) new facilities and diagnostics to study TNE in turbulent flows (iv) extremely scalable codes to conduct massive simulations of turbulence under TNE conditions, (v) detailed measurement of shock-turbulence interactions using Mach stems.

Contents

1 Introduction

1.1 Motivation and objectives

The importance of properly accounting for internal molecular structure of gaseous flows is well established across a number of disciplines including high-temperature aerodynamics and combustion. Utilizing internal energy exchange for intelligent control of basic fluid dynamic processes is of direct relevance to AFOSR scientific objectives (Schmisseur, 2012). The few studies available (see Sec. 1.2) demonstrate a clear link between the internal molecular structure and the basic structure of the fluid dynamic processes, highlighting the extremely limited knowledge about these phenomena which is especially true for strongly non-linear systems like high-Reynolds-number Navier-Stokes turbulence where complexities go beyond any theoretical treatment. The scarce data available has suggested that the interaction mechanisms include both changes in the transport coefficients (e.g. Liao *et al.*, 2010) and coupling of thermal effects into pressure fluctuations (Bowersox & North, 2010). In addition, our recent experimental and numerical results show that turbulence can be generated by thermal non-equilibrium (TNE) and that a drastic decrease of turbulence fluctuations in the streamwise direction can be realized when an RF-plasma is introduced in a turbulent channel flow. Improving understanding and modeling of these mechanisms are scientific challenges that have the potential to lead to new opportunities to extract fluid energy and to control the basic underlying processes. Providing this knowledge is the objective of this proposal, and will ultimately lead to improved thermal management, combustion efficiency and transport prediction. Thus, **the long-term scientific objective** of this project is to take advantage of the fundamental understanding of the transfer of energy between turbulence modes (i.e. kinetic or internal energy) and different molecular internal modes (i.e. rotational, vibrational, electronic) to control and predict the behavior of turbulence over a range of degrees of thermal and mechanical non-equilibrium.

This project aimed at both advancing our understanding of the effect of thermal (mainly vibrational) and mechanical non-equilibrium on compressible turbulence and proposing new technological advances in the mechanisms to generate and control turbulence. Due to the multidisciplinary nature of the problem, multiple approaches have been combined. This project thus included expertise in the fields of large-scale simulations of turbulent flows and atomistic chemical dynamics, physics of turbulence, advanced optical diagnostics, laser-based photochemical TNE generation, and chemistry of non-equilibrium phenomena.

We have investigated a new concept to generate turbulence using photo-initiated TNE mechanisms which we will then use to study the specific mechanisms in which TNE modifies turbulence. The basic principle behind this method is to use a high-energy laser to photoexcite seeded molecules along a mesh pattern. Advantages of this technique include the possibility of selecting molecular species to control the degree and mode of TNE, ease of changing grid geometry, and initial perturbation. A schematic of the laser grid concept is shown in Fig. 1(a). In Fig. 1(b) we show how the photofragment (atomic oxygen) velocity distribution from NO_2 photodissociation aligns with the laser polarization. Fig. 1(c) and (d) compare initial concentration of high-energy fragments (NO) from experiments and simulations, respectively. Lastly, (e) and (f) show the evolution of the turbulent kinetic energy and Reynolds number from preliminary large-scale DNS. The details of findings in this evolution are described in Sec. 3.3 and Sec. 3.4.

Studies were conducted in canonical flows (temporally or spatially decaying turbulence, channel flows and shock-turbulence interactions) with special emphasis on discovering venues to control over which modes energy can be stored—this includes characterizing time and length scales associated with those processes, the relaxation processes from molecular simulations as well as the overall analysis of the underlying coupling mechanisms. At the same time, to compare with baseline cases, equilibrium turbulence simulations and experiments were conducted. The results allowed us to shed

light on long standing inconsistencies between experiments and simulations, such as amplification factors across a shock, or the influence of turbulence scales upstream of the interaction.

(a)

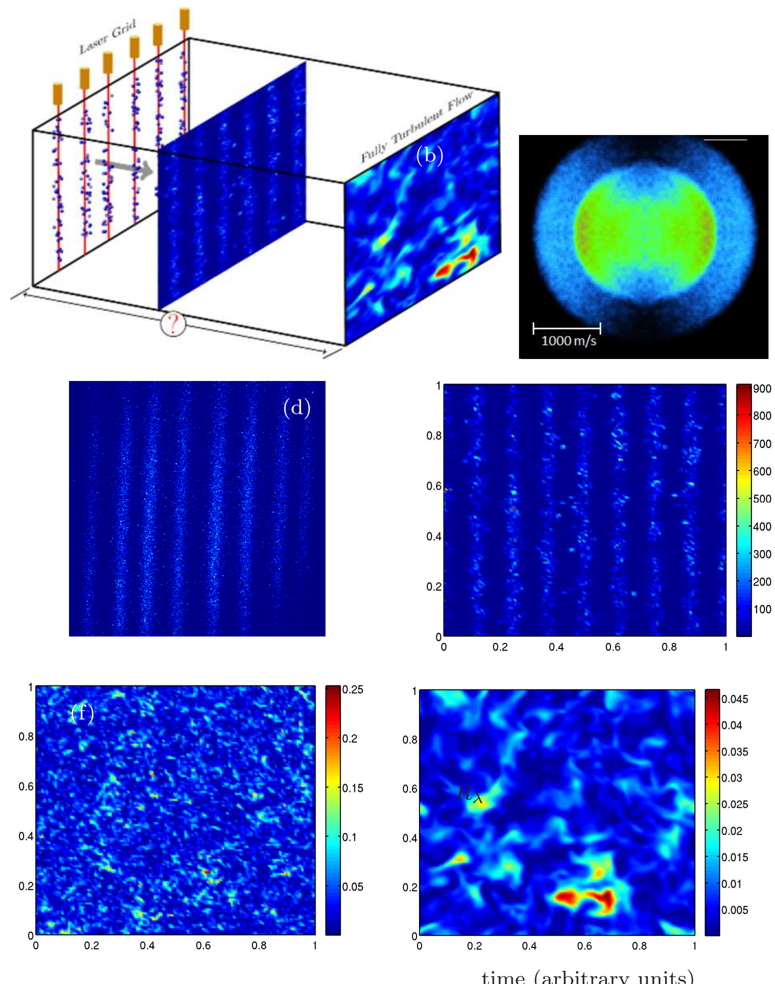

Figure 1: Laser induced non-equilibrium (LINE) turbulence. (a) Schematic of the process. (b) velocity distribution of atomic oxygen after photolysis. (c) and (d) initial distribution of high-energy fragments from experiments and DNS simulations. (e)-(f) contours of turbulent kinetic energy at a time shortly after dissociation took place (d), at an intermediate time $t \approx 1.8$ (e) and at $t \approx 6$ (f) where turbulence is already developed.

As presented in the original proposal, the deliverables of this project included (i) new physical and numerical database and associated analyses with the goal of improved understanding of the intricate connections between thermal and mechanical non-equilibrium and the role thereof in the transport of turbulence (ii) development and characterization of a novel "laser grid" concept based on photolysis to generate turbulence which has the potential to revolutionize turbulence studies in high-speed flows, (iii) development of extremely scalable codes to conduct massive shock-resolving direct numerical simulations of shock-turbulence interactions with TNE at conditions not possible before (iv) first ever detailed measurement of shock-turbulence interactions including TNE effects using Mach stems, and (v) create a multidisciplinary educational environment for PhD students.

While the main focus was on the basic mechanisms for energy exchanges and interplay between

internal degrees of freedom and turbulence, advances are expected to have an impact (i) the science of turbulence (ii) development of turbulence models that can represent more complex scenarios (iii) development of atomistic models to represent complex environments (iv) the frontiers of computational science through code development towards Peta- (and not too far into the future Hexa-) scale computing, and (v) experimental techniques to generate, measure and control both turbulence and non-equilibrium processes.

1.2 Background

A fundamental understanding of the physics involved in turbulence when subjected to thermal and mechanical non-equilibrium is necessary for the development of future supersonic aircraft and weapons, to characterize and control aerothermal environments around control surfaces for missiles and hypersonic vehicles, and for advances in combustion processes.

Detailed gas-dynamic (kinetics) treatises can be found in the texts by Clark & McChesney (1964); Vincenti & Kruger (1975); Chapman & Cowling (1991); Anderson (1990). Related computational studies (J-H., 1985; Deiwert & Candler, 1989; Gnoffo *et al.*, 1989; Park, 1990; Walters *et al.*, 1992; Scalabrin & Boyd, 2005) have provided valuable tools for prediction. However, important computational limitations exist, which ultimately lead to reduced fidelity modeling in both the molecular internal degrees of freedom and the direct resolution of turbulence. The relentless increase in computational power over the last decades, however, has made very large simulations possible. Direct numerical simulations (DNS), which aim at solving all dynamically relevant scales have also been extensively used to study the details of turbulent flows (Moin & Mahesh, 1998; Ishihara *et al.*, 2009) where additional computational power is typically used to push the Reynolds number in fundamental studies of turbulence.

Molecular energy exchange has been the subject of considerable study. The possibilities for treating the internal degrees of freedom range from the case where all the internal modes are in equilibrium with the external mode, that is, a one temperature model, to treating each quantum state of each species as an individual species. There exists in the literature a number of examples of intermediate possibilities. Ultimately, the final conservation law equation set depends on the choice of model fidelity and the functional forms of the energy exchange mechanisms (i.e., the coupling terms) between the energy pools. Descriptions of the underlying physical turbulent processes at the lowest level (i.e. in thermodynamic equilibrium) and the development of engineering models can be found in numerous texts (e.g. Tennekes & Lumley, 1972; Frisch, 1995; Pope, 2000).

While rare in spite of its importance, studies of hydrodynamics interacting with TNE have shown a direct interaction between these processes. Among them, we mention the studies of (i) the effect of thermal non-equilibrium TNE on the stability of boundary layers (Bertolotti, 1998), (ii) the delay of transition from laminar to turbulent flow via vibrational exchange (Fujii & Hornung, 2003), (iii) the effect of rotational/vibrational energy pump in the so-called thermal explosions (Osipov *et al.*, 1999; Uvarov *et al.*, 2002), and (iv) the effect of rotational non-equilibrium on basic statistics of low Reynolds number isotropic turbulence (Liao *et al.*, 2010). We note that only the latter deals with fully turbulent flows.

The rest of the report is organized as follow. In Sec. 2 we present the salient key elements in terms of simulations and experiments that needed to be developed, designed or construtcted in order to achieve our scientific goals. In Sec. 3, we present the highlights of our findings in our investigation of turbulence with TNE. These include studies of fundamental exchanges (at the macro and microscopic label) as well as detailed studies of the LINE concept presented above. Our results on turbulence with mechanical non-equilibrium are described in Sec. **??**.

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